

Wronskian Approach and the One-dimensional Schrödinger Equation with Double-well Potential

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Abstract

A Wronskian determinant approach is suggested to study the energy and the wave function for one-dimensional Schrödinger equation. An integral equation and the corresponding Green's function are constructed. As an example, we employed this approach to study the problem of double-well potential with strong coupling. A series expansion of ground state energy up to the second order approximation of iterative procedure is given.

keywords: double-well potential, Wronskian determinant

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I. INTRODUCTION

As a typical bound-state tunnelling problem, the solutions of one-dimensional Schrödinger equation with double-well potential are of interest and have attracted much attention[1-9]. Recently, Friedberg, Lee and Zhao(FLZ) suggested a new method[7-9] to decide the wave functions of Schrödinger equation by quadrature along a single trajectory. They gave a good trial wave function for double-well potential and constructed the Green's function. By means of the Green's function and the trial wave function, they solved the integral equation by iterative procedure and found the successive approximations for the true wave function and the corresponding energy. They proved that the iterative solution is convergent and gave the numerical result of the ground-state energy at first order approximation of iterative procedure.

The objective of this paper is to address another method, namely, the Wronskian determinant approach(WDA) to study this problem. We will give an integral equation and the Green's function by a general argument. In a specific case, our equation reduces to that equation given by FLZ method. We will solve our integral equation by iterative procedure up to the second order and give the numerical result of the energy. As a comparison, we will use the trial wave function given by ref.[9] and the variational method to calculate the ground state energy. The numerical results given by the three methods(FLZ, WDA and variational method) are quite similar, the differences occur in the higher orders only. This result confirms that the Wronskian determinant approach is also successful for studying the solutions of one-dimensional Schrödinger equation.

II. WRONSKIAN DETERMINANT APPROACH

Consider a second order ordinary differential equation:

$$y'' + p(x)y' + q(x)y = f(x) \quad x \in [a, b] \quad (1)$$

with the boundary conditions:

$$\alpha y(a) + \beta y'(a) = 0 \quad \gamma y(b) + \delta y'(b) = 0 \quad (2)$$

Assume y_1 is a solution of the corresponding homogeneous equation:

$$y'' + p(x)y' + q(x)y = 0 \quad (3)$$

One can easily prove that another linearly independent solution of Eq.(3) reads:

$$y_2 = y_1 \int_a^x y_1^{-2} \Delta dx \quad (4)$$

where $\Delta = \begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix}$ is the Wronskian determinant and it satisfies:

$$\Delta(x) = \Delta(a) \exp\left(-\int_a^x p(x)dx\right) \quad (5)$$

Obviously, y_2 does not satisfy the boundary conditions, because it must satisfy the uniqueness theorem. Suppose the solution y of Eq.(1) can be written as:

$$y = C_1(x)y_1 + C_2(x)y_2 \quad (6)$$

where $C_1(x)$ and $C_2(x)$ are two unknown functions which satisfy a constraint:

$$C_1'(x)y_1 + C_2'(x)y_2 = 0 \quad (7)$$

Since y_2 does not satisfy the boundary conditions, in order that y satisfy Eq.(2), we have:

$$C_2(a) = C_2(b) = 0 \quad (8)$$

Substituting Eq.(6) and Eq.(7) into Eq.(1), noting that y_1 and y_2 are the solution of Eq.(3), we find:

$$C_1'(x)y_1' + C_2'(x)y_2' = f(x) \quad (9)$$

Combining Eq.(7) and Eq.(9), we get:

$$\begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix} \begin{pmatrix} C_1' \\ C_2' \end{pmatrix} = \begin{pmatrix} 0 \\ f(x) \end{pmatrix} \quad (10)$$

Hence:

$$\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \int \begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix}^{-1} \begin{pmatrix} 0 \\ f(x) \end{pmatrix} dx \quad (11)$$

$$C_1 = - \int_B^x \frac{1}{\Delta} y_2 f(x) dx \quad (12)$$

$$C_2 = \int_A^x \frac{1}{\Delta} y_1 f(x) dx \quad (13)$$

$$y = -y_1 \int_B^x \frac{1}{\Delta} y_2 f(x) dx + y_2 \int_A^x \frac{1}{\Delta} y_1 f(x) dx \quad (14)$$

where A and B are two constants. From the identities Eq.(8), we have:

1. The integraton bound $A=a$
2. The integration:

$$\int_a^b \frac{1}{\Delta} y_1 f(x) dx = 0 \quad (15)$$

Eq.(15) is called the 'resonant condition'.

The integral bound 'B' is still undetermined. We will discuss this problem in the next section.

III. SCHRÖDINGER EQUATION

The one-dimensional Schrödinger equation reads:

$$-\frac{1}{2} \frac{d^2}{dx^2} \Phi + V\Phi = E\Phi \quad (16)$$

The boundary conditions for bound-states are:

$$\Phi(\infty) = \Phi(-\infty) = 0 \quad (17)$$

Consider a perturbation equation:

$$-\frac{1}{2} \frac{d^2}{dx^2} \Psi + (V + \omega)\Psi = (E + e)\Psi \quad (18)$$

where ω is the perturbation potential and e the energy shift. Now we study how to find the bound-state wave function Ψ and the energy $E + e$ provided Φ and E are known. The boundary conditions for Ψ reads:

$$\Psi(\infty) = \Psi(-\infty) = 0 \quad (19)$$

Rewrite Eq.(18) as:

$$-\frac{1}{2} \frac{d^2}{dx^2} \Psi + (V - E)\Psi = (e - \omega)\Psi \quad (20)$$

and take the right hand side of Eq.(20) as the inhomogeneous term. By using Eq.(14), we have:

$$\Psi = -2\Phi \int_B^x \Phi_1(\omega - e)\Psi dx + 2\Phi_1 \int_{-\infty}^x \Phi(\omega - e)\Psi dx \quad (21)$$

where $\Phi_1 = \Phi \int_0^x \Phi^{-2} dx$, according to Eq.(4) The resonant condition now becomes:

$$\int_{-\infty}^{\infty} \Phi(\omega - e)\Psi dx = 0 \quad (22)$$

We can get the energy shift by the identity Eq.(22) if Ψ is obtained. However, the lower bound B of the integral in Eq.(21) is undetermined. Notice that the different choices of B will only lead to an extra constant times Φ in Eq.(21). Then we can fix B=0 and rewrite Eq.(21) as:

$$\Psi = c\Phi - 2\Phi \int_0^x \Phi_1(\omega - e)\Psi dx + 2\Phi_1 \int_{-\infty}^x \Phi(\omega - e)\Psi dx \quad (23)$$

Combine the two integrations (using Eq.(22)):

$$\Psi = c\Phi - 2\Phi \int_0^x \Phi^{-2}(y) dy \int_y^{\infty} \Phi(z)(\omega - e)\Psi(z) dz \quad (24)$$

There are two ways to determine the constant c :

- (i) Assume that the perturbation potential is zero at infinity, then $\frac{\Phi(\infty)}{\Psi(\infty)} = 1$, and according to Eq.(24):

$$1 = \frac{\Psi(\infty)}{\Phi(\infty)} = c - 2 \int_0^\infty \Phi^{-2}(y) dy \int_y^\infty \Phi(z)(\omega - e)\Psi(z) dz \quad (25)$$

Substitute Eq.(25) back into Eq.(24), we have:

$$\Psi = \Phi - 2\Phi \int_\infty^x \Phi^{-2}(y) dy \int_y^\infty \Phi(z)(\omega - e)\Psi(z) dz \quad (26)$$

This is the result given by FLZ method[9].

- (ii) The integral equation can be solved by iterative method, using $\Psi_0 = \Phi$ as the zeroth approximation, the corresponding energy shift is:

$$e_1 = \frac{\int_{-\infty}^\infty \Phi^2 \omega dx}{\int_{-\infty}^\infty \Phi^2 dx} \quad (27)$$

according to Eq.(22). The first approximation of wave function Ψ_1 is given by:

$$\Psi_1 = c_0 \Phi - 2\Phi \int_0^x \Phi^{-2}(y) dy \int_y^\infty \Phi(z)(\omega - e_1)\Phi(z) dz \quad (28)$$

Put $c_0 = 1 + N$, where N is chosen to be:

$$N = \frac{2 \int_{-\infty}^\infty \Phi^2 dx \int_0^x \Phi^{-2}(y) dy \int_y^\infty \Phi(z)(\omega - e_1)\Phi(z) dz}{\int_{-\infty}^\infty \Phi^2 dx} \quad (29)$$

we choose c_0 to satisfy:

$$\langle \Psi_1 | \Phi \rangle = \langle \Phi | \Phi \rangle \quad (30)$$

which means the modification $(\Psi_1 - \Phi)$ is orthorgonal to Φ . Similarly, e_2 is given by:

$$e_2 = \frac{\int_{-\infty}^\infty \Phi \Psi_1 \omega dx}{\int_{-\infty}^\infty \Phi \Psi_1 dx} \quad (31)$$

and the corresponding constant c_1 is chosen to satisfy:

$$\langle \Psi_2 | \Phi \rangle = \langle \Phi | \Phi \rangle \quad (32)$$

and so on. This method of choosing c features that c is different in each order of iterative procedure and the modification of each order is orthorgonal to Φ .

IV. DOUBLE-WELL POTENTIAL

As an example, we will employ the wronskian determinant approach to discuss the one-dimensional Schrödinger equation with double-well potential. Schrödinger equation reads:

$$-\frac{1}{2} \frac{d^2}{dx^2} \Psi + \frac{1}{2} g^2 (x^2 - 1)^2 \Psi = E \Psi \quad (33)$$

where g is a large parameter in the strong coupling case.

Since the potential is symmetric, we can solve it in the half space $x \geq 0$ only. So the boundary condition for the ground state becomes:

$$\Psi(\infty) = \Psi'(0) = 0 \quad (34)$$

The trial wave function given by ref.[9] is:

$$\Phi = \frac{1}{1+x} \exp\left(-\frac{g}{3}(x-1)^2(x+2)\right) \quad (35)$$

The derivative of Φ is not zero at the origin. We must do some modification. Let:

$$\tilde{\Phi} = \begin{cases} \Phi + \frac{g-1}{g+1} \exp\left(-\frac{4g}{3}\right) \exp\left(\frac{g}{3}(x-1)^2(x+2)\right) & \text{for } 0 < x < 1 \\ \Phi + \frac{g-1}{g+1} \exp\left(-\frac{4g}{3}\right) \Phi & \text{for } x > 1 \end{cases} \quad (36)$$

The difference between $\tilde{\Phi}$ and Φ is of the order $\exp\left(-\frac{4g}{3}\right)$. For strong coupling, $g \gg 1$, the difference is exponentially small and can be neglected. We can still choose Φ as our trial function. the wave function Φ satisfies:

$$-\frac{1}{2} \frac{d^2}{dx^2} \Phi + \left(\frac{1}{2} g^2 (x^2 - 1)^2 + \frac{1}{(1+x)^2}\right) \Phi = g \Phi \quad (37)$$

Treat this equation as the unperturbed one, and $-\frac{1}{(1+x)^2}$ as the perturbative potential ω . Employing the Wronsky determinant approach, the integral equation reads:

$$\Psi = c\Phi - 2\Phi \int_0^x \Phi^{-2}(y) dy \int_y^\infty \Phi(z)(\omega - e)\Psi(z) dz \quad (38)$$

The energy shift is given by:

$$e = \frac{\int_0^\infty \Phi \Psi \omega dx}{\int_0^\infty \Phi \Psi dx} \quad (39)$$

We solve the integral equation Eq.(38) by iterative procedure.

A. First order approximation

At the first order approximation, $\Psi_0 = \Phi$, the energy shift e_1 and the Ψ_1 are:

$$e_1 = \frac{\int_0^\infty -\frac{1}{(1+x)^4} \exp(-\frac{2g}{3}(x-1)^2(x+2))dx}{\int_0^\infty \frac{1}{(1+x)^2} \exp(-\frac{2g}{3}(x-1)^2(x+2))dx} \quad (40)$$

$$\Psi_1 = (1+N)\Phi - 2\Phi \int_1^x \Phi^{-2}(y)dy \int_y^\infty \Phi(z)(\omega - e)\Phi(z)dz \quad (41)$$

where we have put the integration lower bound to be 1 instead of 0. The difference can be cancelled by the modification of N . This alteration will bring some convenience in the calculation. N is also chosen to satisfy:

$$\langle \Psi_1 | \Phi \rangle = \langle \Phi | \Phi \rangle \quad (42)$$

For strong coupling, $g \gg 1$, using the integral formula:

$$\int_{-a}^a f(x) \exp(-gx^2)dx \sim f(0)\sqrt{\frac{2\pi}{g}} + \frac{f''(0)}{4}\sqrt{2\pi}g^{-3/2} + \dots + f^{(2n)}(0)\frac{\Gamma(\frac{2n+1}{2})}{(2n)!}g^{-n-\frac{1}{2}}\dots \quad (43)$$

we obtain a series of $1/g$ for energy:

$$e_1 = -\frac{1}{4} - \frac{9}{64}g^{-1} - 0.1660g^{-2} - 0.2755g^{-3}\dots$$

and

$$E = g - \frac{1}{4} - \frac{9}{64}g^{-1} - 0.1660g^{-2} - 0.2755g^{-3}\dots$$

by a straight calculation.

B. Second order approximation

At the second order approximation, the energy shift e_2 is:

$$e_2 = \frac{(1+N) \int_0^\infty \Phi \omega \Phi dx - 2 \int_0^\infty \Phi \omega \Phi dx \int_1^x \Phi^{-2}(y)dy \int_y^\infty \Phi(z)(\omega - e_1)\Phi(z)dz}{\int_0^\infty \Phi^2 dx} \quad (44)$$

We are facing on the triple integration in the numerator of Eq.(44). The detailed calculation of the triple integration is presented in the appendix. The result is:

$$e_2 = -\frac{1}{4} - \frac{9}{64}g^{-1} - 0.1738g^{-2} - 0.3107g^{-3}\dots$$

and

$$E = g - \frac{1}{4} - \frac{9}{64}g^{-1} - 0.1738g^{-2} - 0.3107g^{-3}\dots$$

C. Variational Method

In this section, we use another method, namely, variational method, to calculate the ground state energy. The trial function is chosen as:

$$\Phi = \frac{1}{1+x} \exp\left(-\frac{f}{3}(x-1)^2(x+2)\right) \quad (45)$$

where f is the variational parameter. The ground state energy is:

$$E = \frac{\int_0^\infty \left[\frac{f}{(1+x)^2} - \frac{1}{(1+x)^4} + \frac{1}{2}(g^2 - f^2)(x-1)^2 \right] \exp\left(-\frac{2f}{3}(x-1)^2(x+2)\right) dx}{\int_0^\infty \frac{1}{(1+x)^2} \exp\left(-\frac{2f}{3}(x-1)^2(x+2)\right) dx} \quad (46)$$

The integration in both the numerator and denominator of Eq.(46) can be calculated by using Eq.(43). The result is:

$$f = g - \frac{9}{64}g^{-1} - 0.3320g^{-2} - 0.8366g^{-3} \dots$$

and

$$E = g - \frac{1}{4} - \frac{9}{64}g^{-1} - 0.1660g^{-2} - 0.2855g^{-3} - 0.6184g^{-4} \dots$$

V. DISCUSSION AND CONCLUSION

In summary, we have studied the ground state energy and the wave function by using the WDA. We have found that the Green's function and the integral equation are the same as that of FLZ method provided the integral lower bound B and parameter c are chosen as ∞ and 1 respectively. we suggest a method to determine parameter c which warrant that the modification of Φ is orthogonal to Φ , which is similar to the general perturbation method. We have expanded the energy as a series of g^{-1} for double-well potential and obtained:

$$E = g - \frac{1}{4} - \frac{9}{64}g^{-1} - 0.1660g^{-2} - 0.2755g^{-3} \dots \quad (1st \text{ order iterative approximation})$$

$$E = g - \frac{1}{4} - \frac{9}{64}g^{-1} - 0.1738g^{-2} - 0.3107g^{-3} \dots \quad (2nd \text{ order iterative approximation})$$

$$E = g - \frac{1}{4} - \frac{9}{64}g^{-1} - 0.1660g^{-2} - 0.2855g^{-3} \dots \quad (variational \text{ method})$$

The three results are quite similar to each other up to the order $O(g^{-1})$. It is confirmed that the WDA is a successful method to investigate the one-dimensional Schrödinger equation and the alternative way of determining the parameter c is reasonable. The differences of energy between different methods and approximations occur at the order of g^{-2} and higher terms.

VI. APPENDIX

We will calculate the triple integration:

$$\int_0^\infty \Phi \omega \Phi dx \int_1^x \Phi^{-2}(y) dy \int_y^\infty \Phi(z)(\omega - e_1) \Phi(z) dz \quad (47)$$

Let $u := x - 1$, the integration becomes:

$$\begin{aligned} & \int_{-1}^\infty \Phi \omega \Phi(u) du \int_0^u \Phi^{-2}(v) dv \int_v^\infty \Phi(w)(\omega - e_1) \Phi(w) dw \\ &= - \int_{-1}^\infty \frac{1}{(2+u)^4} \exp(-2g(u^2 + u^3/3)) du \int_0^u (2+v)^2 \exp(2g(v^2 + v^3/3)) dv \\ & \quad \int_v^\infty \frac{1}{(2+w)^2} (\omega - e_1) \exp(-2g(w^2 + w^3/3)) dw \\ &= \int_0^\infty \dots \int_0^u \dots \int_v^\infty \dots + \int_{-1}^0 \dots \int_0^u \dots \int_v^\infty \dots \end{aligned} \quad (48)$$

which is the Lagrange's inverse function theorem.

Suppose function $x = f(z)$ is analytic at the region: $|z - z_0| < \rho, -\pi + \delta < \arg(z - z_0) < \pi - \delta$:

$$f(z) = f(z_0) + a_k(z - z_0)^k + a_{k+1}(z - z_0)^{k+1} + \dots$$

while $\varphi(z)$ is analytic in the neighbourhood of z_0 . Then:

$$\varphi(z) = \varphi(z_0) + \sum_1^n \frac{1}{n!} \frac{d^{n-1}}{dx^{n-1}} [\varphi'(z) \left(\frac{z - z_0}{(f(z) - f(z_0))^{1/k}} \right)^n] \Big|_{z=z_0} (x - x_0)^{n/k} \quad (49)$$

where $x_0 = f(z_0)$.

When $\varphi(z) = z$, Eq.(49) gives the formulae of inverse function $z = f^{-1}(x)$. In our case, Let:

$$x = u^2 + u^3/3$$

We find:

$$\frac{1}{(u+2)^2} = 1/4 - \frac{1}{4}x^{1/2} + \frac{11}{48}x \dots \quad (50)$$

$$\frac{1}{(u+2)^4} = 1/16 - \frac{1}{8}x^{1/2} + \frac{17}{96}x \dots \quad (51)$$

$$du = \left(\frac{1}{2}x^{-1/2} - 1/6 + \frac{5}{48}x^{1/2} \dots \right) dx \quad (52)$$

Eqs.(50)~(52) are only valid for $u > 0$. When $u < 0$, they can be calculated similarly. Thus the first part of Eq.(48) becomes:

$$\int_0^\infty (1/16 - \frac{1}{8}x^{1/2})(\frac{1}{2}x^{-1/2} - 1/6) \exp(-2gx)dx \int_0^x (4 + 4y^{1/2})(\frac{1}{2}y^{-1/2} - 1/6) \exp(2gy)dy \int_y^\infty (1/4 - \frac{1}{4}z^{1/2})(-1/4 + \frac{1}{4}z^{1/2} - e_1)(\frac{1}{2}z^{-1/2} - 1/6) \exp(-2gz)dz \quad (53)$$

The problem now is reduced to the calculating of the standard form:

$$\int_0^\infty x^{m/2} \exp(-2gx)dx \int_0^x y^{n/2} \exp(2gy)dy \int_y^\infty z^{p/2} \exp(-2gz)dz \quad (54)$$

where m, n, p are integers ranging from -1 to infinity.

Rewrite Eq.(54) as:

$$\int_0^\infty x^{m/2} \exp(-2gx)dx \int_0^x y^{n/2} \exp(2gy)dy \int_x^\infty z^{p/2} \exp(-2gz)dz + \int_0^\infty x^{m/2} \exp(-2gx)dx \int_0^x y^{n/2} \exp(2gy)dy \int_y^x z^{p/2} \exp(-2gz)dz \quad (55)$$

In the first part, let: $x = zs, y = zst, z = z$ $s \in [0, 1]$ $t \in [0, 1]$ and $J = \left| \frac{\partial(x,y,z)}{\partial(z,s,t)} \right| = z^2 s$

In the second part, let: $x = x, y = xst, z = xs$ $s \in [0, 1]$ $t \in [0, 1]$ and $J = \left| \frac{\partial(x,y,z)}{\partial(x,s,t)} \right| = x^2 s$
Eq.(55) becomes:

$$\int_{D_1} s^{\frac{m+n+2}{2}} t^{n/2} z^{\frac{m+n+p+4}{2}} \exp[-2gz(1-st+s)] dz ds dt + \int_{D_2} s^{\frac{m+p+2}{2}} t^{n/2} x^{\frac{m+n+p+4}{2}} \exp[-2gx(1-st+s)] dx ds dt \quad (56)$$

where

$$D_1 : z \in [0, \infty), s \in [0, 1], t \in [0, 1] \quad (57)$$

$$D_2 : x \in [0, \infty), s \in [0, 1], t \in [0, 1] \quad (58)$$

The variables x and z can be integrated Eq.(56) becomes:

$$\frac{\Gamma(\frac{m+n+p+6}{2})}{(2g)^{(m+n+p+6)/2}} \int s^{\frac{m+n+2}{2}} t^{n/2} z^{\frac{m+n+p+4}{2}} (1-st+s)^{-\frac{m+n+p+6}{2}} ds dt + \frac{\Gamma(\frac{m+n+p+6}{2})}{(2g)^{(m+n+p+6)/2}} \int s^{\frac{m+p+2}{2}} t^{n/2} x^{\frac{m+n+p+4}{2}} (1-st+s)^{-\frac{m+n+p+6}{2}} ds dt \quad (59)$$

Now the parameter g is extracted out, the remaining two double integrations are independent of g and the area for integration is a rectangle, they can be calculated easily.

We calculate the integration which satisfy $\frac{m+n+p+6}{2} \leq k$ and sum all these integrations, it will give us the first part of Eq.(48). The second part can be calculated with the same procedure.

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